Propanoic acid, 2-(1-oxopropoxy)-, methyl ester 61402-72-0 | DTXSID30485366

61402-72-0 D1XSID30485366	

Model Performance

N.A. I. I.	D .
Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 198 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

Image not found

Propylene glycol diacetate

Measured: 191 Predicted: 198

Image not found

Diethyl propanedioate

Measured: 200 Predicted: 206

Image not found

Butanedioic acid, ethyl methyl

ester

Measured: 208 Predicted: 206

Image not found

1,3-Propanediol, diacetate

Measured: 210 Predicted: 206